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Precision NNLO determination of $\alpha_s(M_Z)$ using an unbiased global parton set

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Abstract:

We determine the strong coupling α_s at NNLO in perturbative QCD using the global dataset input to the NNPDF2.1 NNLO parton fit: data from neutral and charged current deep-inelastic scattering, Drell-Yan, vector boson production and inclusive jets. We find $\alpha_s(M_Z) = 0.1173 \pm 0.0007^{\text{stat}}$, where the statistical uncertainty comes from the underlying data and uncertainties due to the analysis procedure are negligible. We show that the distribution of α_s values preferred by different experiments in the global fit is statistically consistent, without need for rescaling uncertainties by a “tolerance” factor. We show that if deep-inelastic data only are used, the best-fit value of α_s is somewhat lower, but consistent within one sigma with the global determination. We find that the shift between the NLO and NNLO values of α_s is $\Delta\alpha_s^{\text{pert}} = 0.0018$, and we estimate the uncertainty from higher-order corrections to be $\Delta\alpha_s^{\text{NNLO}} \sim 0.0009$.

We have recently shown [1] that a surprisingly precise determination of α_s using next-to-leading order perturbative QCD can be obtained from the dependence on the value of the strong coupling of the quality of a global unbiased fit [2] of parton distributions to deep-inelastic, Drell-Yan and inclusive jet data. This result was somewhat unexpected. Indeed, previous determinations of α_s from global parton fits based on the idea of treating α_s as a fit parameter [3–5] obtained larger uncertainties, and the precision of Ref. [1] is achieved even though the underlying PDF parametrization [2] adopted there is so general that the concept of a global best fit is no longer useful, and one must instead consider the fit quality (as measured by the χ^2) as a Monte Carlo random variable which only stabilizes in the limit of very large Monte Carlo sample size.

Given the great interest of an accurate determination of α_s , in particular for Higgs searches at the LHC [6], it is important to repeat the analysis of Ref. [1] at NNLO, i.e. using the most accurate available QCD theory. This is the purpose of this study: besides determining α_s and providing a detailed assessment of statistical and procedural uncertainties, and a general discussion of its reliability, we will provide an estimate of residual theoretical uncertainties.

Our methodology is the same as in Ref. [1], to which we refer for a more detailed discussion. Here, it will be sufficient to recall that our determination is based on exploiting the fact that parton distributions determined with the NNPDF methodology [7–12] are delivered for several values of α_s , with all other aspects of the analysis being kept fixed. The quality of the fit of the data, as measured by its χ^2 , can then be determined for each value of α_s . Because NNPDF parton distributions are delivered as a set of Monte Carlo replicas, the χ^2 is a random variable, whose fluctuations only tend to zero in the limit of large sample size (as explicitly verified in Ref. [1]). The expected standard deviation of the χ^2 for given sample size can be determined using the bootstrap method, as discussed in Ref. [1]. We thus arrive at a determination of the χ^2 curve as a function of α_s for a discrete set of values of α_s and with an accuracy which depends on the size of the Monte Carlo replica sample. Both the set of values of α_s and the sample size can then be enlarged, until satisfactory accuracy is reached.

In Ref. [1] this was done by suitably enlarging both the number of values of α_s and number of replicas of the available NNPDF2.1 NLO parton distribution sets [13]. Here, we start with the NNPDF2.1 NNLO parton distributions [2], which are available for $\alpha_s(M_Z)$ in the range from 0.114 to 0.124 in steps of 0.001, with $N_{\text{rep}} = 1000$ replicas for $\alpha_s(M_Z) = 0.119$, and $N_{\text{rep}} = 100$ replicas for all other values. We have extended this range down to 0.110, and we have considerably increased the number of available replicas: we eventually end up with the number of replicas and values of α_s summarized in Table 1.

The χ^2 values obtained for each value of α_s are shown in Fig. 1; the total number

Values of $\alpha_s(M_Z)$	N_{rep}
0.114,0.115,0.116,0.117,0.118,0.119	1000
0.112,0.113,0.120,0.121	500
0.110,0.111,0.122,0.123,0.124	100

Table 1: The number of PDF replicas N_{rep} in the PDF set for each value of $\alpha_s(M_Z)$.

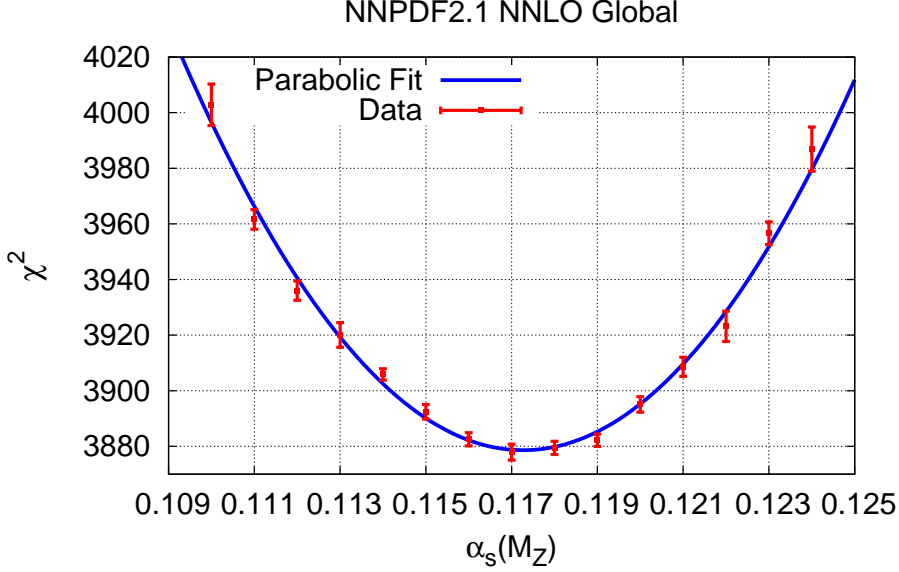


Figure 1: The χ^2 as a function of α_s using NNLO NNPDF2.1 parton distributions. The uncertainty shown is due to the finite size of the PDF replica sample used to compute the χ^2 for each value of α_s . The curve is the result of a parabolic fit.

of data points is $N_{\text{dat}} = 3357$ [2], and at the minimum $\chi^2/N_{\text{dat}} = 1.16$. The error bar shown on each point is the standard deviation determined using the bootstrap method as described in Ref. [1]. A parabolic fit leads to

$$\alpha_s^{\text{NNLO}}(M_Z) = 0.1173 \pm 0.0007^{\text{stat}} \pm 0.0001^{\text{proc}}, \quad (1)$$

where the statistical uncertainty corresponds to a shift by one from the minimum of the parabola, while the procedural uncertainty is propagated from the finite-size uncertainty on the χ^2 values, and it is clearly completely negligible. The χ^2 per degree of freedom of the parabolic fit shown in Fig. 1 is $\chi^2_{\text{par}}/N_{\text{dof}} = 1.1$. This value remains unchanged if the outer two or four points are removed from the parabolic fit: this means that the behaviour of the curve shown is parabolic to within the accuracy of the individual points.

Equation (1) is the main result of this paper. It is interesting to compare this to the NLO result of Ref. [1], namely

$$\alpha_s^{\text{NLO}}(M_Z) = 0.1191 \pm 0.0006^{\text{stat}} \pm 0.0001^{\text{proc}}, \quad (2)$$

which was obtained using exactly the same methodology, from PDFs in turn determined using the same methodology and the same data ¹; the value of the χ^2 per data point at the minimum at NLO is also the same, namely $\chi^2/N_{\text{dat}} = 1.16$. The result appears to be perturbatively quite stable. The small difference in statistical error between the NLO

¹The number of datapoints for the NLO fit of Ref. [1] is $N_{\text{dat}} = 3338$ [13]: the slightly lower number of datapoints in the NLO case is due to the fact that the kinematic cuts on charm structure function data must be more stringent at NLO in order to exclude data for which NNLO corrections are very large, as discussed in more detail in Ref. [2].

Experiment	α_s	σ^{stat}	σ^{proc}	σ^{tot}	P	χ^2/N_{dof}
NMCpd	0.1146	0.0105	0.0019	0.0107	-0.25	0.5
NMCp	0.1150	0.0020	0.0003	0.0020	-1.06	1.6
BCDMS	0.1158	0.0014	0.0002	0.0015	-0.92	1.2
HERA-I	0.1199	0.0019	0.0002	0.0019	1.31	1.0
ZEUS-H2	0.1231	0.0030	0.0002	0.0030	1.89	0.9
NuTeV	0.1177	0.0038	0.0004	0.0039	0.10	1.2
CDFZRAP	0.1205	0.0074	0.0033	0.0081	0.40	1.2
CDFR2KT	0.1225	0.0021	0.0003	0.0021	2.35	1.8
D0R2CON	0.1111	0.0028	0.0004	0.0029	-2.10	0.5

Table 2: The best-fit values of α_s obtained from a parabolic fit to the χ^2 profiles of Fig. 2. Only experiments for which the parabola has a minimum in the fitted range are included. In each case we also show the statistical and procedural uncertainties (defined as in Eq. (1)), their sum in quadrature σ^{tot} , the pull P Eq. (3), and the χ^2 of the parabolic fit.

and NNLO fits indicates that the NLO fit quality deteriorates slightly faster when moving away from the minimum. However, this difference does not appear to be statistically significant: the gaussian uncertainty on the uncertainty is $\sigma_\sigma = \sigma/\sqrt{2N}$, which in our case, with $\sigma = 0.0007$ and $N = N_{\text{dof}}$ (the number of degrees of freedom of the parabolic fit) is $\sigma_\sigma = 0.0001$.

The statistical uncertainty on the determination of α_s Eq. (1) is very small when compared to the uncertainty on other existing determinations of α_s : for example, the statistical uncertainty on the NNLO MSTW determination [3], which is also based on a PDF fit to a similar set of data, is twice as large. The size of the uncertainty on the MSTW08 result is significantly affected by the fact that a tolerance [14] criterion is used to obtain 68% confidence levels. This means that uncertainty ranges in parameter space are rescaled by an amount which is determined by requiring a reasonable behaviour of the distribution of best-fit results for the various parameters among the different experiments that enter the global fit, whose fluctuations may be significantly larger than expected on the basis of unrescaled uncertainties. It is thus important to establish whether such a rescaling is also necessary in our case.

We do this (as in Ref. [1]) using a variant of the method suggested in Ref. [15]. Namely, we determine that the distribution of results obtained from individual datasets follows a Gaussian distribution. A possible deviation from unity of the width of this distribution would then indicate the need for tolerance rescaling. Of course care should be taken that α_s values obtained from individual experiments in a global fit are correlated by the underlying global fit; these correlations could in principle lead to spurious minima in the χ^2 profile which would be absent if α_s was fitted from that experiment only, and thus would be of no significance.

We have thus determined the profile of the contribution to the χ^2 of the global fit from each experiment entering the global NNPDF2.1 NNLO determination: all profiles are displayed in Fig. 2, along with their NLO counterparts of Ref. [1]. We have then determined α_s and its uncertainty from a parabolic fit to each profile. For each experiment whose parabola has a minimum in the fitted range we have determined the pull, defined

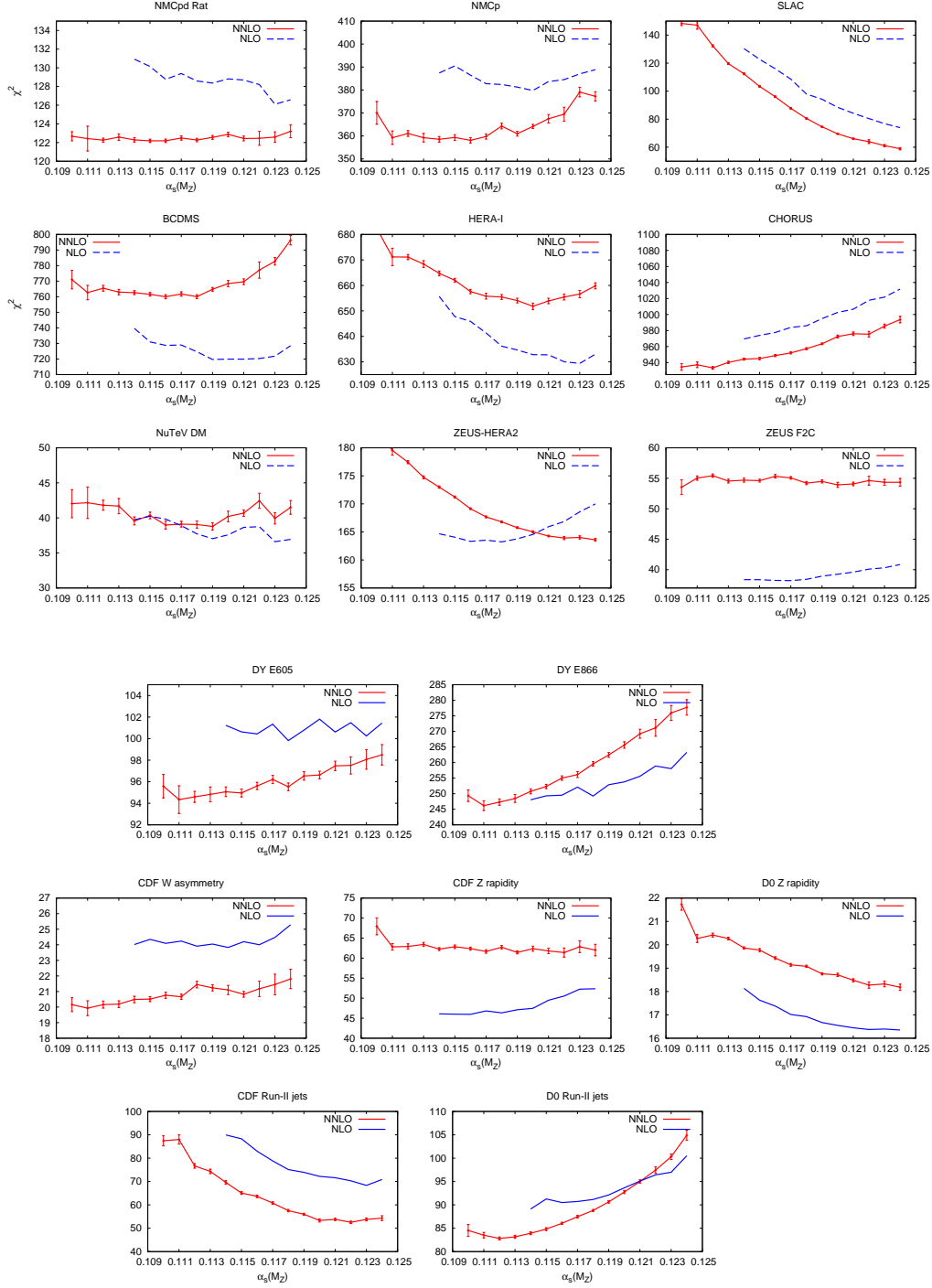


Figure 2: Contribution to the total χ^2 from each experiment entering the NNPDF2.1 NNLO PDF determination, plotted as a function of α_s , including the uncertainty on each point due to the finite size of the replica sample. The NNPDF2.1 NLO curves from Ref. [1] are also shown.

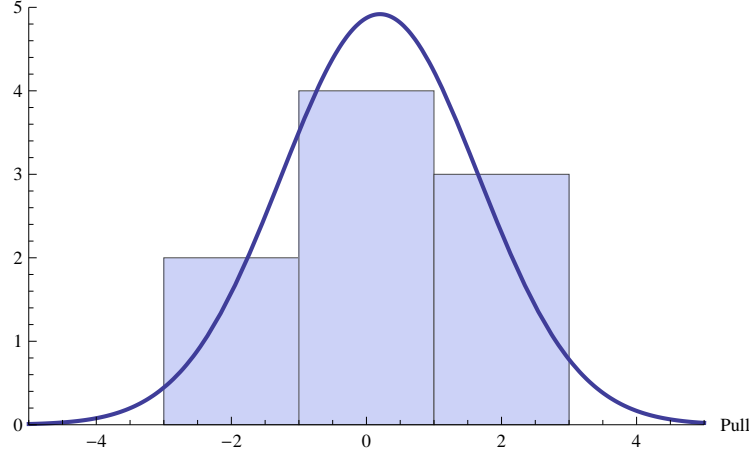


Figure 3: Histogram of the distribution of pulls included in Table 2, together with a gaussian fit to it.

as

$$P_i \equiv \frac{\alpha_s^{(i)}(M_Z) - \alpha_s(M_Z)}{\sqrt{(\sigma_{(i)}^{\text{tot}})^2 + (\sigma^{\text{tot}})^2}}, \quad (3)$$

where $\alpha_s(M_Z)$ is the global best-fit value Eq. (1) and $\sigma^{\text{tot}} = \sqrt{(\sigma^{\text{stat}})^2 + (\sigma^{\text{proc}})^2}$ the uncertainty on it determined from the statistical and procedural uncertainties also of Eq. (1), while $\alpha_s^{(i)}(M_Z)$ and $\sigma_{(i)}^{\text{tot}}$ are the corresponding values for the i -th experiment. The best-fit value, statistical and procedural uncertainty for the i -th experiment are determined by applying to the χ^2 profile for the contribution of the i -th experiment to the global fit exactly the same procedure used for the determination of the corresponding quantities in the global fit, and they are thus subject to the caveat that correlations with other experiments are neglected (for example, procedural uncertainties in each individual experiment will now have point-by-point correlation due to other experiments included in the global fit).

The best-fit values of α_s , uncertainties and pulls are collected in Table 2, along with the χ^2 of the parabolic fit to each individual profile.² Clearly for some datasets (such as NMCpd or CDFZRAP) the minimum is actually quite shallow, as apparent from Figure 2, and the uncertainty in Table 2 is correspondingly large: these data would not by themselves provide a determination of α_s . However, note that here we are not determining the best-fit α_s from each dataset, but rather studying the compatibility of different data sets within the global fit: from this point of view, data with a shallow minimum or no minimum are certainly compatible, and thus not problematic.

The pull distribution has mean and standard deviation

$$\langle P \rangle = 0.19 \pm 0.33; \quad \sigma_P = 1.46 \pm 0.24, \quad (4)$$

²Note that the definition of pull Eq. (3) is the same as in Eq. (3) of Ref. [1], however all pulls were incorrectly given in Table 3 of that reference with the opposite sign convention.

where the uncertainties on the mean and standard deviation are computed assuming that the population of nine pulls is extracted from a univariate Gaussian distribution. In Fig. 3 the histogram of the pull distribution is compared to a Gaussian normalized to the area under the histogram, and with mean and width given by Eq. (4). We conclude that the pull distribution is consistent, with either no need or minimal need for tolerance rescaling. Even if one were to rescale the statistical uncertainty on α_s by the pull, one would end up with a statistical uncertainty of 0.0010 instead of 0.0007.

Having established that the estimate of the statistical uncertainty in our main result Eq. (1) is robust, we now turn to the issue of theoretical uncertainties. The main theoretical uncertainty comes from higher order QCD corrections. An indication of its size can be obtained by comparing results obtained at subsequent perturbative orders. Our NNLO and NLO results, Eqs. (1) and (2) respectively, differ by

$$\Delta\alpha_s^{\text{pert}} \equiv |\alpha_s^{\text{NNLO}} - \alpha_s^{\text{NLO}}| = 0.0018. \quad (5)$$

This is likely to provide an upper bound to the uncertainty on the NNLO determination from higher order corrections. Hence, the perturbative stability of our result suggests that the higher order uncertainty on it is quite small.

A somewhat less crude estimate can be obtained using a method recently proposed in Ref. [16], based on the idea that a Bayesian estimate of the behaviour of unknown higher orders of a perturbative series can be obtained from the behaviour of the known orders. The 68% confidence level (i.e. one sigma) uncertainty Δ_k due to higher order corrections to the k -th order result

$$\sigma_k = c_l \alpha_s^l + c_{l+1} \alpha_s^{l+1} + \dots + c_k \alpha_s^k \quad (6)$$

under the assumptions of the model in Ref. [16] is then given by

$$\Delta_k = \begin{cases} \alpha_s^{k+1} \max\{|c_l|, \dots, |c_k|\} \frac{n_c+1}{n_c} 0.68 & \text{if } 0.68 \leq \frac{n_c}{n_c+1} \\ \alpha_s^{k+1} \max\{|c_l|, \dots, |c_k|\} [(n_c+1)0.32]^{-1/n_c} & \text{if } 0.68 > \frac{n_c}{n_c+1}, \end{cases} \quad (7)$$

with $n_c = k+1-l$ the number of known perturbative coefficients.

In our case, the output value of α_s in our analysis is not determined from the perturbative expansion of a single quantity, but rather from the expansion for all processes which enter the global PDF fit. However, we can obtain an estimate for its perturbative behaviour by letting

$$\alpha_s^{\text{fit}}(M_Z) = \sum_{k=0}^{\infty} c_k [\alpha_s^0(M_Z)]^k \quad (8)$$

where α_s^{fit} is the result of our determination at a given perturbative order, while α_s^0 is some underlying input “true” value of the strong coupling. We then know the values of α_s^{fit} at NLO and NNLO, but we do not know the value of α_s^{fit} at LO, nor the input value α_s^0 . We obtain our estimate by varying both in a wide range: we take $\alpha_s^{\text{fit,LO}} \in [0.100, 0.180]$ and $\alpha_s^0 \in [0.110, 0.125]$ and then we use Eq. (7), with α_s^{fit} Eq. (8) evaluated at NLO or NNLO, and take in each case the largest output value for Δ_k as the input parameters are varied.

We then get

$$\Delta^{\text{NLO}} \equiv \Delta_1 = 0.0077 \quad (9)$$

$$\Delta^{\text{NNLO}} \equiv \Delta_2 = 0.0009, \quad (10)$$

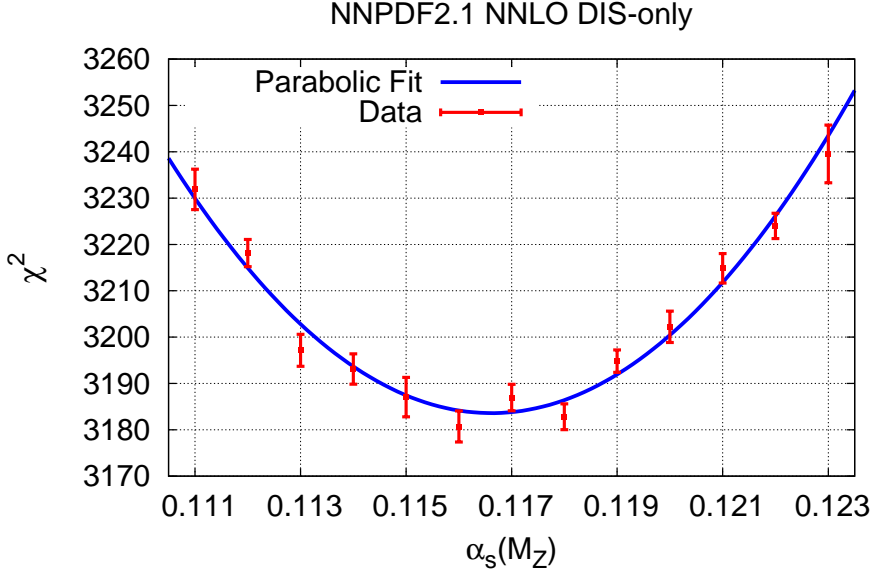


Figure 4: Same as Fig. 1, but using the NNPDF2.1 NNLO DIS only PDF set.

so that in particular the NNLO uncertainty is about half the shift between the NLO and NNLO values. Clearly, results depend significantly on the range of variation of $\alpha_s^{\text{fit,LO}}$: for example, if we restricted it to $\alpha_s^{\text{fit,LO}} \in [0.100, 0.160]$ we would get $\Delta_1 = 0.0053$ and $\Delta_2 = 0.0006$. We have chosen a very broad range in order to obtain a conservative estimate. A more careful assessment could be obtained by performing a similar analysis (or factorization and renormalization scale variation) for each of the processes which enters the global fit, and then combining the ensuing uncertainties, while the analysis given here should be viewed as a semi-quantitative way of putting on a firmer footing the expectation that the uncertainty on α_s at a given order due to higher-order corrections should be a fraction of the shift of the best-fit value of α_s from the previous to the given order.

We thus see that while at NLO theoretical uncertainties arising from higher perturbative orders are dominant over statistical uncertainties, at NNLO the two uncertainties are of similar size, and thus our determination of α_s appears to remain quite accurate even when this uncertainty is included. Of the further sources of theoretical uncertainty, the largest is likely to be related to the treatment of heavy quarks, though such uncertainty is typically [17] smaller than that related to higher order corrections.

A sizable fraction of the data which are used for the NNPDF2.1 PDF determination comes from deep-inelastic scattering experiments. There is a widespread perception (see e.g. [18, 19]) that α_s determinations based on deep-inelastic data lead to a value which is somewhat smaller than the global average. In Ref. [1], we have shown that in a DIS-only fit the BCDMS data (which have been long known [20] to favor a low $\alpha_s \sim 0.114$) have a minimum of the χ^2 at rather low $\alpha_s \lesssim 0.113$. However, this is no longer the case if the BCDMS data are included in a global fit along with Drell-Yan and jet data. We have traced this to the fact that at low α_s DIS data and jet data pull the gluon in opposite directions, so the fit quality can be improved using DIS data only in a way which is

forbidden when jet data are present. Similar results have been obtained in Refs. [21, 22], where it was further argued that this effect is stronger if the gluon parametrization is too restrictive, and it was in fact shown explicitly that within the MSTW fitting framework low NNLO best-fit values (similar or lower to the values $\alpha_s \sim 0.113$ obtained at NNLO in Ref. [4]) are obtained if either the gluon parametrization is more restrictive, or jet data are excluded from the fit. In Ref. [1] we found that in the NNPDF framework (where an extremely flexible PDF parametrization is used) the effect of the BCDMS data on the DIS fit remains moderate: though the BCDMS data favor a low value of α_s , the DIS-only best fit α_s is still $\alpha_s \sim 0.118$, consistent with the global NLO best fit. However, the analysis of Ref. [1] is only performed at NLO, so one is immediately led to ask what happens at NNLO.

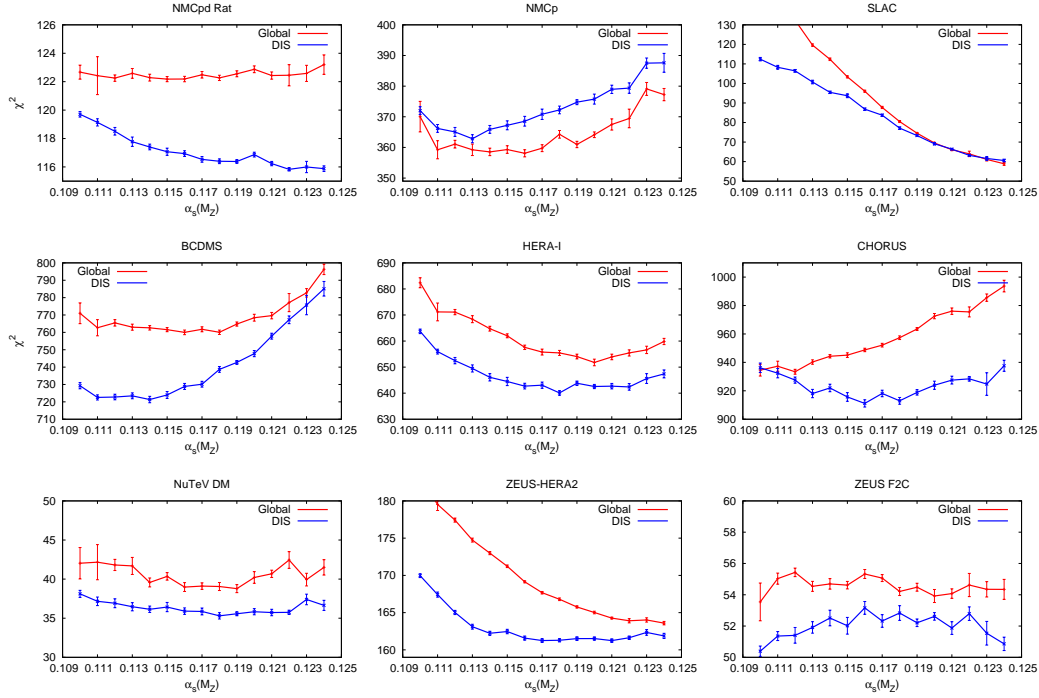


Figure 5: Same as Fig. 2, but now comparing results obtained using the NNLO global and DIS-only fits.

We have thus repeated our NNLO determination of α_s , but now only including deep-inelastic scattering data in the computation of the χ^2 . Starting with the NNPDF2.1 NNLO DIS-only fit of Ref. [2], we have generated $N_{\text{rep}} = 500$ replicas for all values of $\alpha_s(M_Z)$ in the range from 0.110 to 0.124 in steps of 0.001. The χ^2 values and finite-size uncertainties that we get are shown in Fig. 4, to be compared to Fig. 1 of the global fit; the number of data points now is $N_{\text{dat}} = 2783$ [2], and at the minimum $\chi^2/N_{\text{dat}} = 1.14$. A parabolic fit has a $\chi^2_{\text{par}}/N_{\text{dof}} = 1.2$, and leads to

$$\alpha_s^{\text{NNLO}}(M_Z) = 0.1166 \pm 0.0008^{\text{stat}} \pm 0.0001^{\text{proc}}. \quad (11)$$

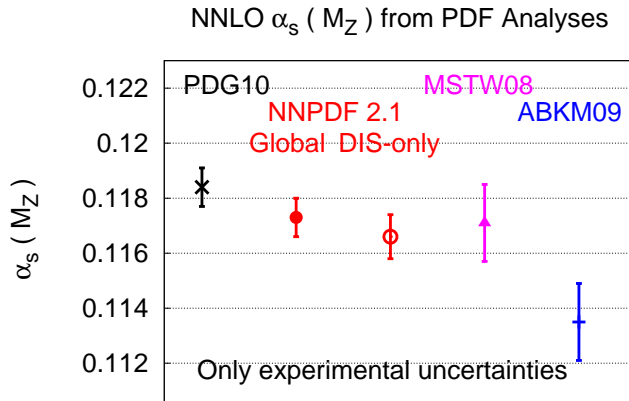


Figure 6: Comparison of the NNPDF2.1 NNLO $\alpha_s(M_Z)$ determinations to other recent determinations from NNLO PDF analysis. The PDG value of Ref. [18] is also shown.

Note that the outer two points at $\alpha_s(M_Z) = 0.110, 0.124$ have not been used, because the quality of the parabolic fit would considerably deteriorate. The χ^2 profiles from individual datasets in the global and DIS-only fit are compared in Fig. 5.

Comparing our global and DIS-only determinations of α_s Eqs. (1) and (11) we see that, like at NLO [1], also at NNLO the DIS-only value, though somewhat smaller than the global one, agrees with it within the (small) statistical uncertainty at the one sigma level. The pattern of χ^2 profiles for individual experiments is also similar at NLO and NNLO: the BCDMS data have a minimum for much lower α_s in the DIS only fit than in the global fit. Note however that the overall DIS-only best-fit value of α_s Eq. (11) remains quite close to the global one, unlike in the MSTW08 case where the NNLO DIS-only value ends up being quite low (0.1139, to be compared to 0.1171 for the global fit) — perhaps because of our especially flexible PDF parametrization. In this respect, it is interesting to observe that MSTW find [21] that their DIS-only result depends strongly on whether the parametrization allows the gluon to become negative or not; in the NNPDF determination positivity is imposed at the level of physical observables, thus leading to a milder constraint on the PDF itself.

Our results for the NNLO α_s determinations, both from the global data set and from DIS data only, are displayed graphically in Fig. 6, where they are also compared to the other recent NNLO ABKM09 [4] and MSTW08 [3] determinations. Our results are in good agreement with MSTW, but with smaller uncertainties. The ABKM result is rather lower, but it should be kept in mind that ABKM only use DIS data and a smaller set of fixed-target Drell-Yan data, with a parton parametrization which is more restrictive than the MSTW one, so it is subject to the caveats mentioned above and discussed in Ref. [21].

In summary, we have presented the most accurate available NNLO α_s determination from a global parton fit. The greater statistical accuracy of our result in comparison to other available determinations of α_s along with PDFs [3, 4] is due both to the use of the particularly flexible and reliable NNPDF approach to PDF parametrization and fitting,

and to the use of a wide and up-to-date dataset (in particular the recent combined HERA data [23] which are not used in Refs. [3, 4]). The theoretical uncertainty on our determination is likely to be dominated by higher-order perturbative QCD corrections, and thus there is no reason why it should be different from any other analogous determination (such as Refs. [3, 4]). This uncertainty has not been determined accurately so far. However, the considerable perturbative stability we find, demonstrated by the moderate shift between our NLO and NNLO results, suggests that it might be smaller than hitherto expected: in particular, our estimate for it is less than half than that provided in Ref. [3]. It will be interesting to repeat this analysis once the very accurate data on standard candle processes from the LHC become available.

Acknowledgments

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